



High-Pressure Supercritical Fuel Injection at Diesel Conditions

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June 7, 2017

Project ID: ACS107



Overview

Timeline

- Project start date: Jan 1, 2016
- Project end date: Dec 31, 2018
- Percent complete: 35%

Budget

- Total project funding
 - \$542,487
 - DOE share: \$476,012
 - Cost share: \$66,475
- Funding received in FY 2016
 - \$165,356
- Funding for FY 2017
 - \$151,895

Barriers

- Lack of modeling capability for combustion and emission control
- Lack of fundamental knowledge of advanced engine combustion regimes
- Lack of effective engine controls

Partners

- Argonne National Laboratory

Project Objectives

- Produce an extensive *experimental data set* to validate CFD models simulating high-pressure diesel fuel spray at supercritical or near *supercritical conditions*.
- Produce a validated *real-fluid property code* which can be integrated with computational fluid dynamics (CFD) solvers.
- Document CFD code modifications needed for supercritical fluid spray simulations using the *Eulerian-Eulerian (EE)* approach.
- Establish the *accuracy assessment* of the EE approach to simulate fuel spray at high-pressure diesel engine operating conditions.
- Support VTO office goal: By 2018, further increase the thermal efficiency of a heavy truck engine to 55 percent which represents about a 30 percent improvement over current engines.
- Project content is aimed directly at the listed barriers.

Project Approach

- **Experiment Setup and Initial Model Development:** Modification and construction of experimental apparatus to support proposed work as well as initial fluid modeling development will proceed in parallel.
- **Baseline Experimental Testing and CFD Integration:** Experimental data will be collected to support model validation in both open source and commercial CFD codes.
- **Parametric Studies in Both CFD and Experiment:** Parametric studies of ambient conditions, fuel injection parameters, and fuel composition will be pursued both experimentally and numerically. The developed models will be integrated into a commercial CFD code and validation and demonstration studies will be performed.

Milestones

| 2017 Milestone | Type | Description |
|---|-----------|--|
| CPFR Fabricated and Operational | Technical | Startup of CPFR demonstrates ability of chamber to reach required design bulk gas conditions |
| Preliminary URANS Calculations Complete | Technical | Preliminary URANS calculations verify integrity of the CFD code |
| Integrate Real Fluid Property Module to Commercial Code | Technical | Implementation of real-fluid property module in commercial code complete |
| ECN Spray A Testing Complete | Technical | Baseline supercritical injection studies complete |
| Validation Method Confirmed | Go/No-Go | RSD accuracy sufficient to serve as quantitative validation for model development |

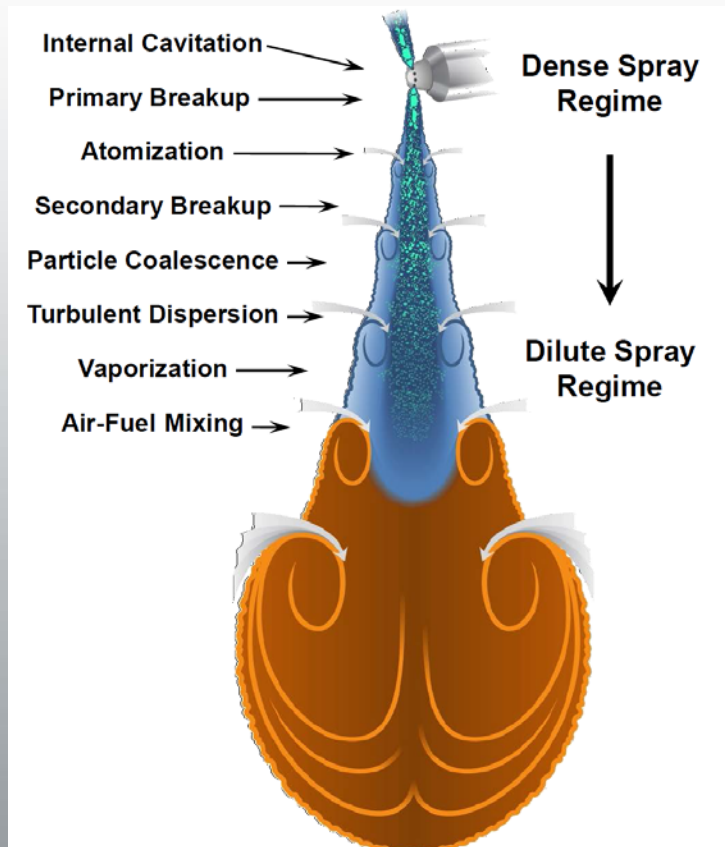
| 2018 Milestone | Type | Description |
|--|-----------|--|
| Baseline Commercial Code | Technical | Validation of integrated CFD code using baseline experimental data complete |
| Pressure and Temperature and Fuel Injector Parametric Studies Complete | Technical | Testing to acquire statistically significant data sets at range of bulk gas conditions and injector resulting in supercritical behavior complete |
| Code Flexibility Validated | Technical | Code flexibility to switch from supercritical to subcritical conditions validated and reacting flow simulations complete |
| Uncertainty Analysis Complete | Technical | Uncertainty analysis on model constants complete |

Project Accomplishments

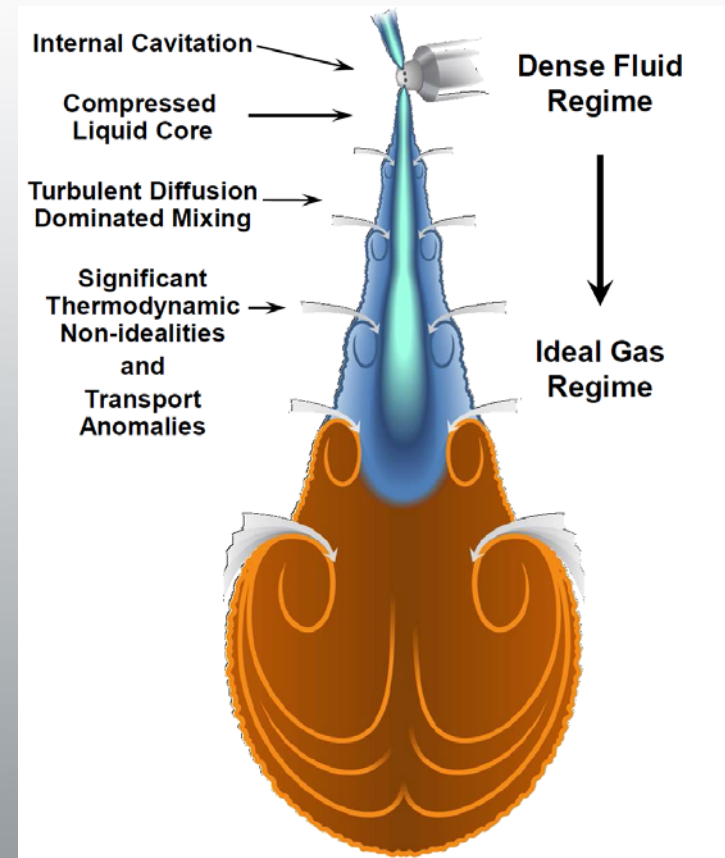
- Developed correlations to compute thermodynamic and transport properties at the high-pressure conditions.
- Developed/validated a stand-alone numerical module to calculate thermo-physical properties based on the selected real-fluid model.
- Optimized high-speed rainbow schlieren deflectometry (RSD) setup for diagnostics in a constant pressure flow rig (CPFR)
- Modified and developed schlieren analysis techniques to obtain equivalence ratio and liquid penetration depth
- Designed/constructed CPFR to simulate supercritical conditions

Differing Spray Regimes

Conventional, Subcritical Processes



Supercritical Processes



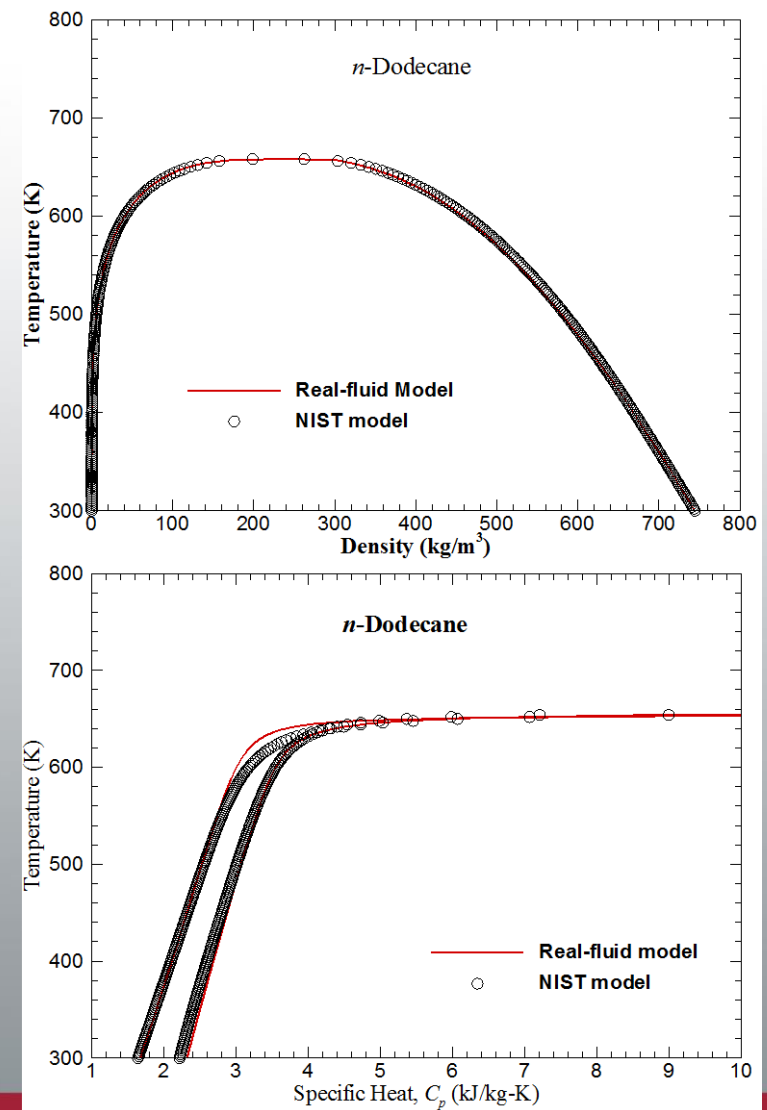
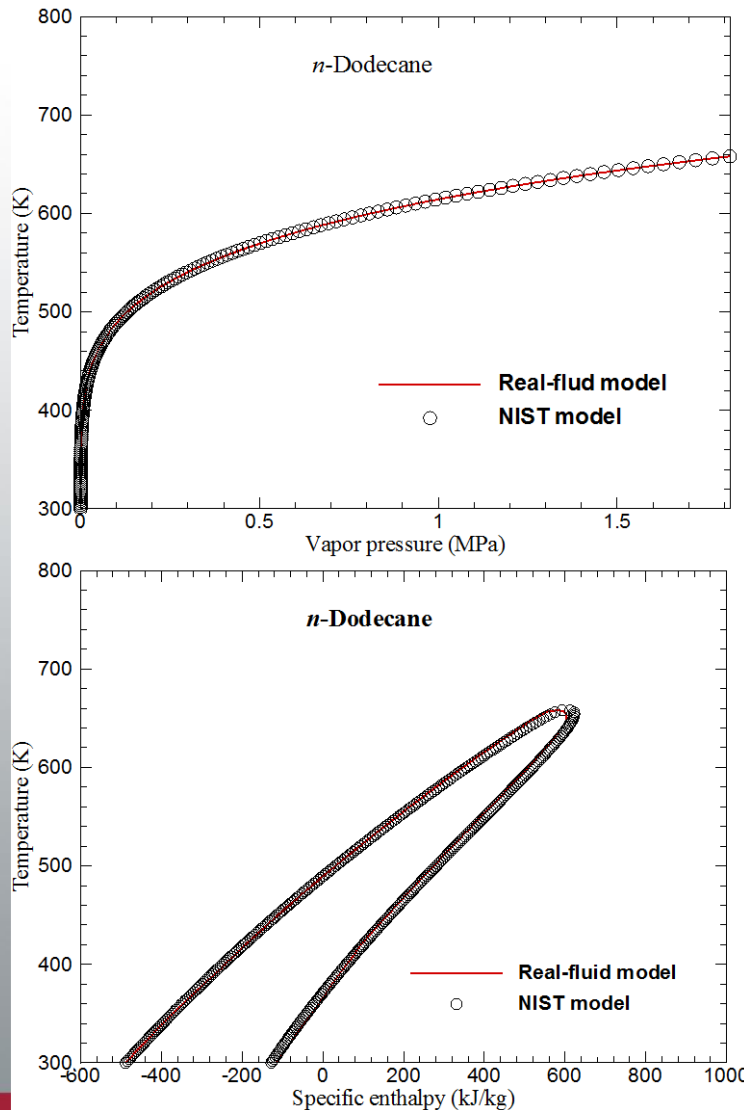
Oefelein, et al, AEC Update 2012

Thermophysical Property Models

- Literature review of various equations of state (EoS) and correlations for estimating thermal and transport properties were completed
- Evaluations of EoS for the thermal properties were performed and completed
- For transport properties:
 - Evaluations of models for viscosity were performed and completed
 - Evaluations of models for thermal conductivity is in progress
 - Evaluations of mass diffusivity models are put on hold because
 - Mass diffusivity of a pure substance is not unique and is highly affected by its neighboring species
 - Theoretical method for mass diffusivity is limited to binary diffusion and gases
 - Development of empirical correlations has been hindered by the complexity of the various possible species surrounding the substance and lack of test data

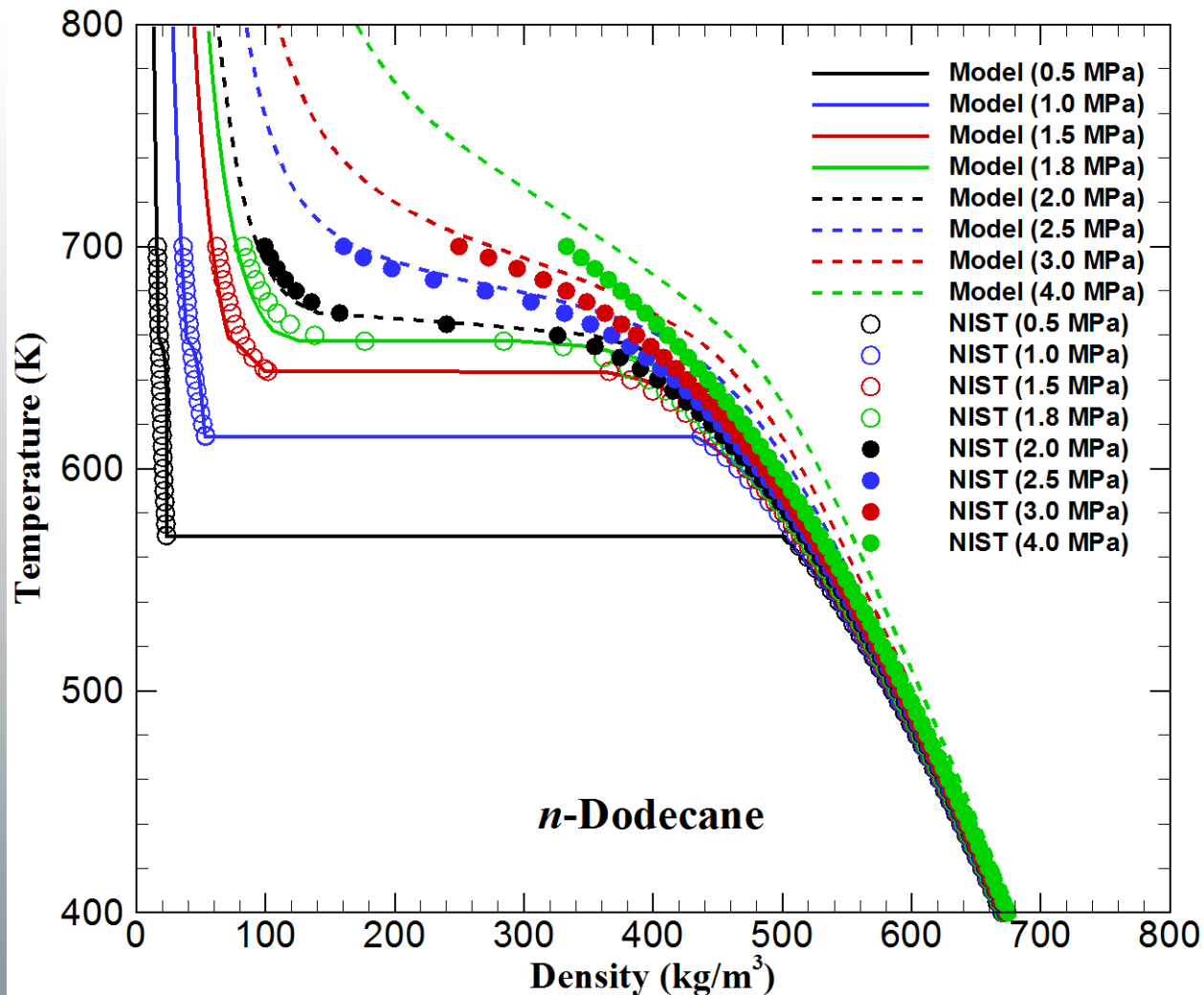
Thermal Properties

Comparison of saturation properties



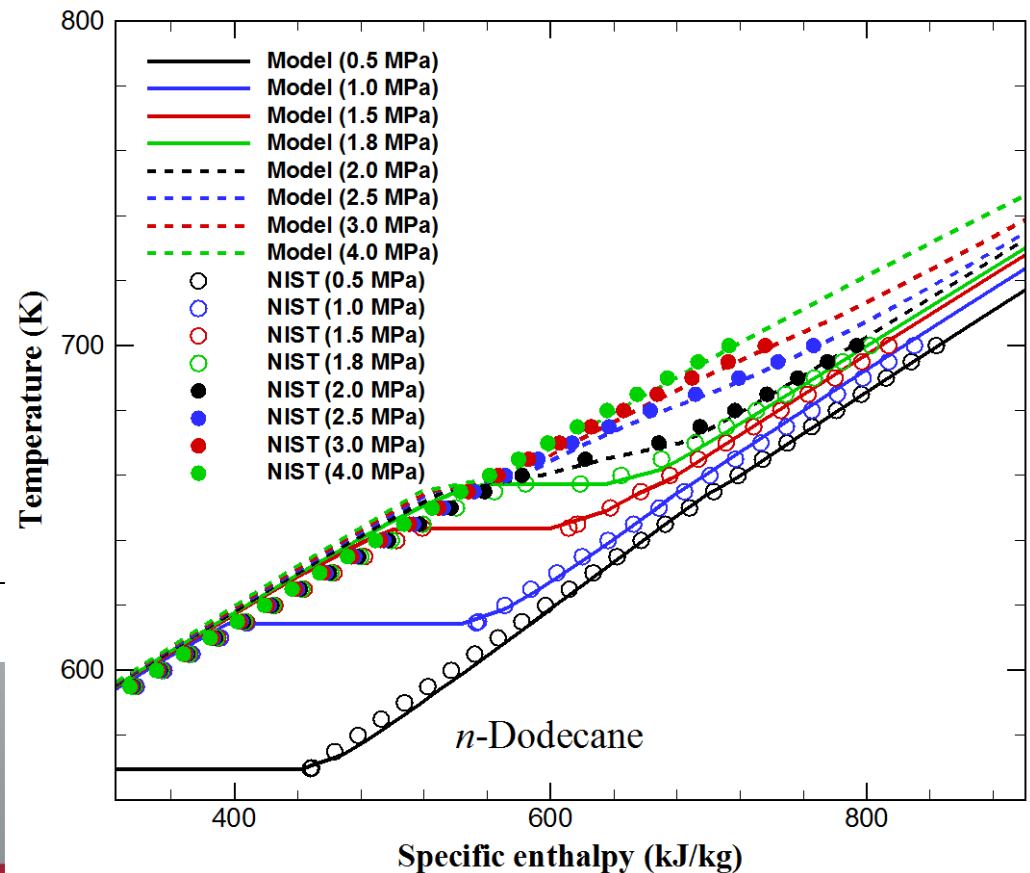
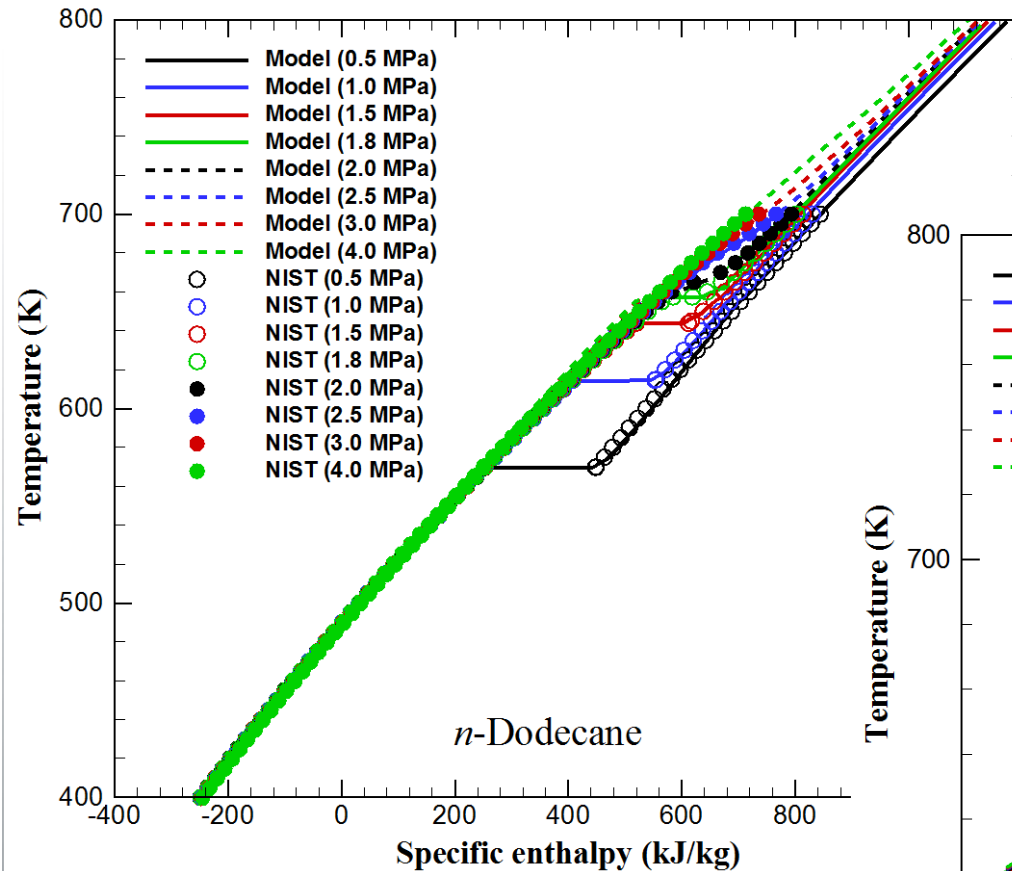
Thermal Properties

Comparison of density-temperature relation



Thermal Properties

Comparison of enthalpy-temperature relation

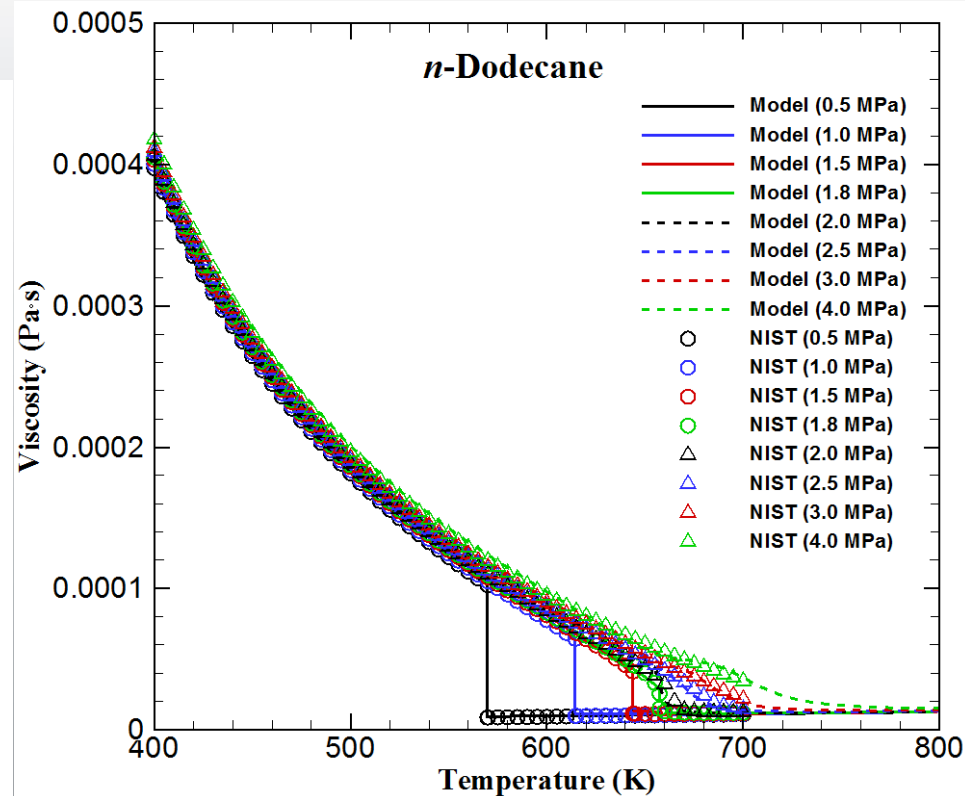
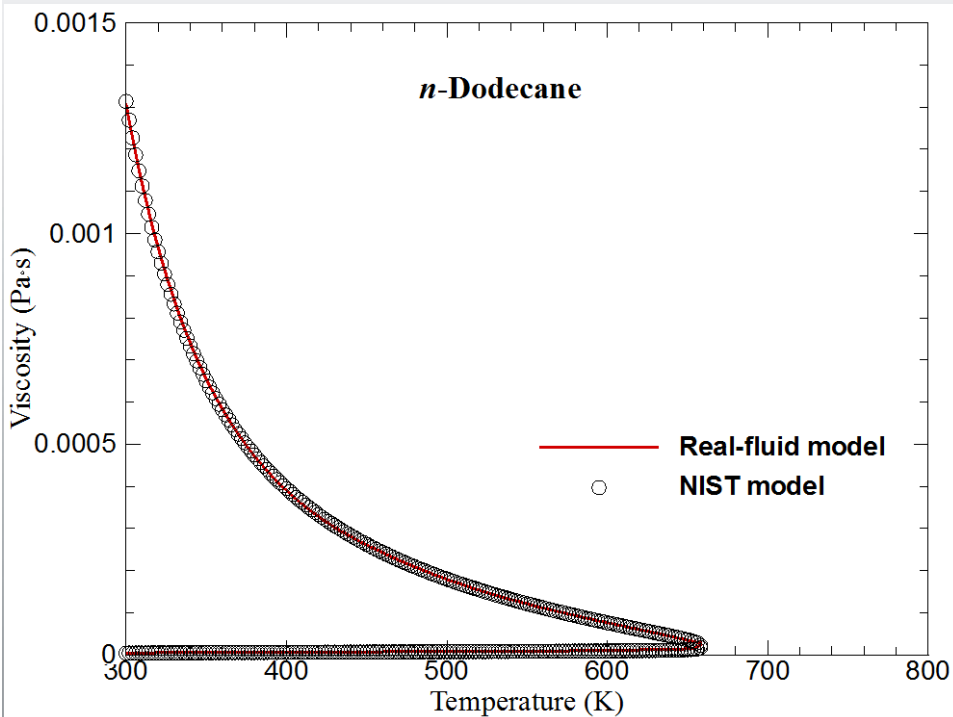


Viscosity

Comparison of Temperature-Viscosity Relation

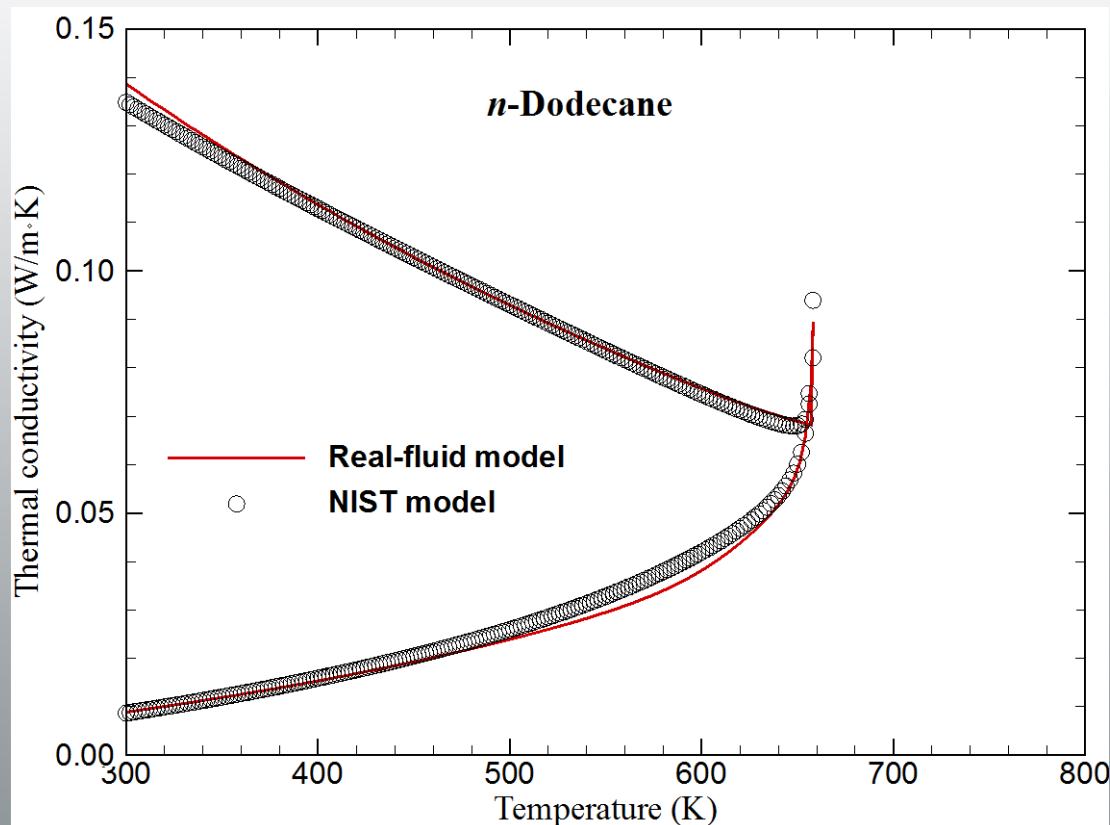
Various Pressures

Saturation Condition



Thermal Conductivity

Comparison of temperature-thermal conductivity relation at saturation condition



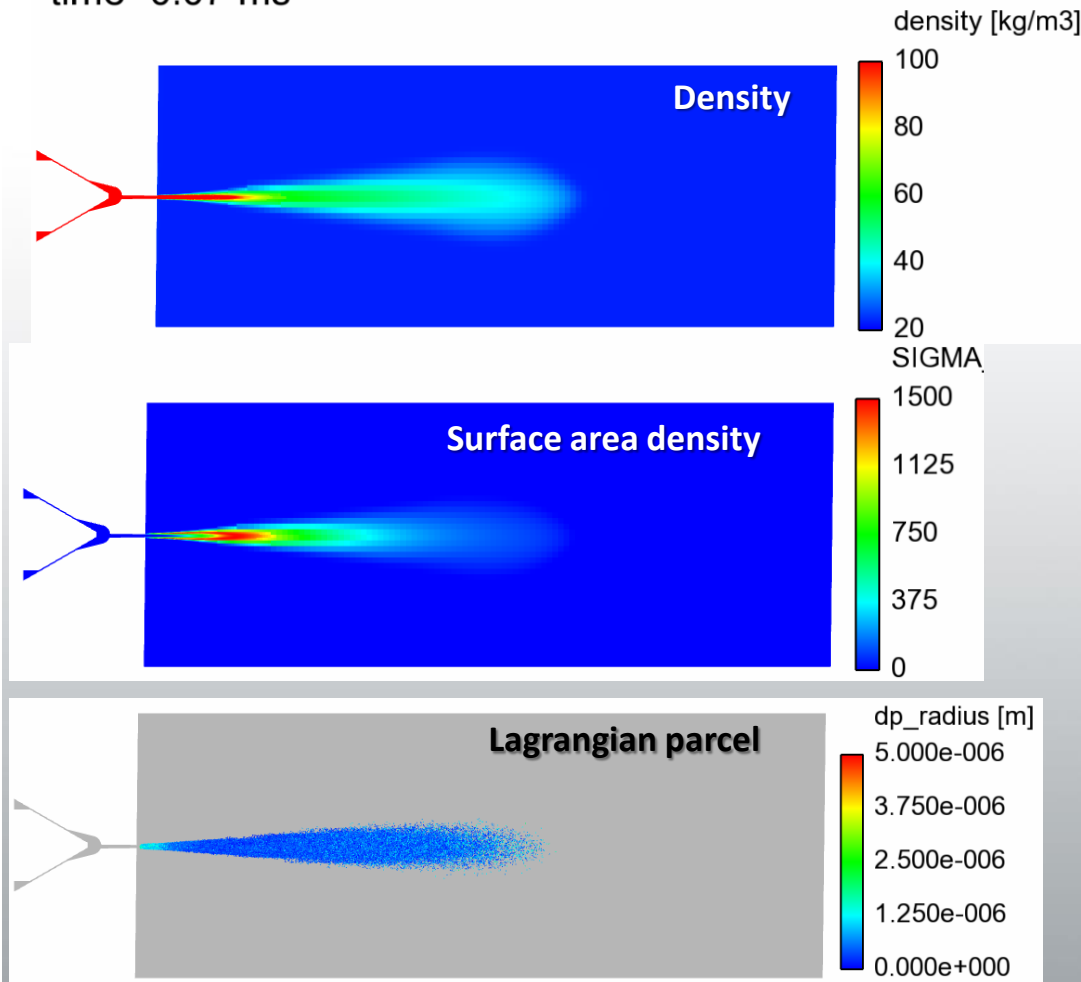
ANL Eulerian-Lagrangian Spray Atomization (ELSA) model for CFD Analysis

- Eulerian approach (Volume of Fluid) for the dense fluid at in-nozzle and near-nozzle region:
 - Effect of in-nozzle flow on spray process is considered;
 - Liquid and gas phase are tracked by individual species equations;
 - Single fluid approach for both sub- and super-critical condition: liquid and gas phase within the same cell have the same value of velocity, temperature and pressure;
 - Void fraction α :
$$\alpha = \frac{m_g/\rho_g}{m_g/\rho_g + m_l/\rho_l} \quad (m: \text{mass}; \rho: \text{density}; g: \text{gas}; l: \text{liquid})$$
 - Surface area density $\tilde{\Sigma}$:
$$\frac{\partial \tilde{\Sigma}}{\partial t} + \nabla \cdot (\tilde{\mathbf{u}} \tilde{\Sigma}) = \nabla \cdot (D_{\Sigma} \nabla \tilde{\Sigma}) + \alpha_1 \frac{\tilde{\varepsilon}}{k} \tilde{\Sigma} \left(1 - \frac{\tilde{\Sigma}}{\tilde{\Sigma}_{eq}}\right) + S_{\Sigma_{evap}} + S_{\Sigma_{init}}$$

(D_{Σ} : diffusivity; α_1 : model constant; $\tilde{\Sigma}_{eq}$: equilibrium value driven by turbulent stretching and coalescence processes; $S_{\Sigma_{evap}}$: source term due to evaporation; $S_{\Sigma_{init}}$: initialization source term)
- Conversion of Eulerian liquid into Lagrangian phase for the diluted spray under sub-critical condition in the downstream region
 - Relatively coarse mesh can be used to achieve efficient computation
 - Transition occurs where the liquid is sufficiently dispersed ($\alpha > 1 - \alpha_{cutoff}$)
- The ELSA model has been developed and validated for engine spray modeling at ANL

Test case for ELSA model under sub-critical condition

time=0.07 ms



- Under sub-critical condition, the injected fuel undergoes primary and secondary breakup processes, followed by classical interphase vaporization. These processes can be modeled by the current ELSA model.
- Under super-critical condition with respect to both pressure and temperature, no distinct phase exists between liquid and gas. The liquid is modeled as continuum Eulerian fluid. The physical model developed at University of Alabama will be used to govern the dense fluid properties.

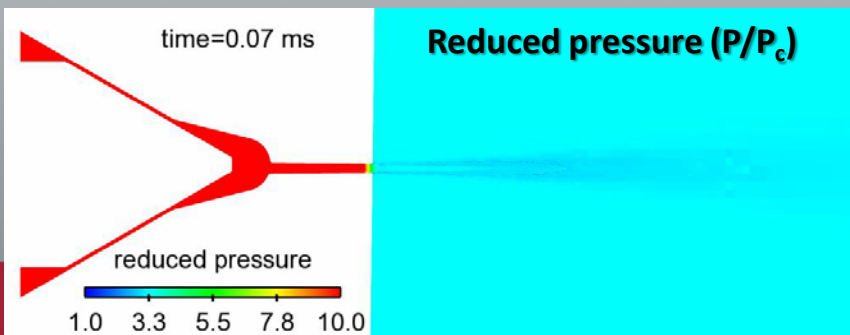
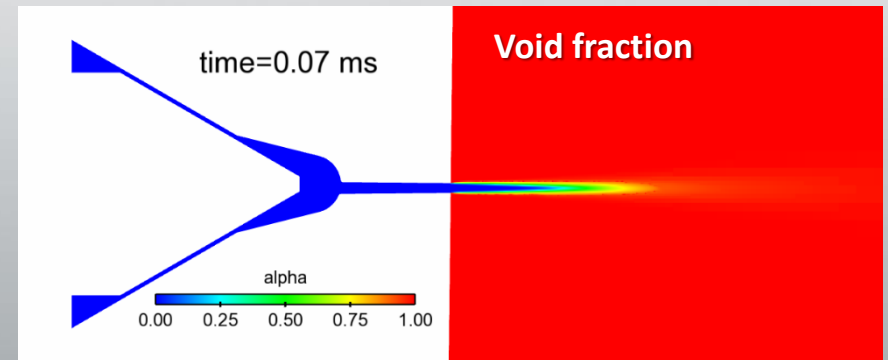
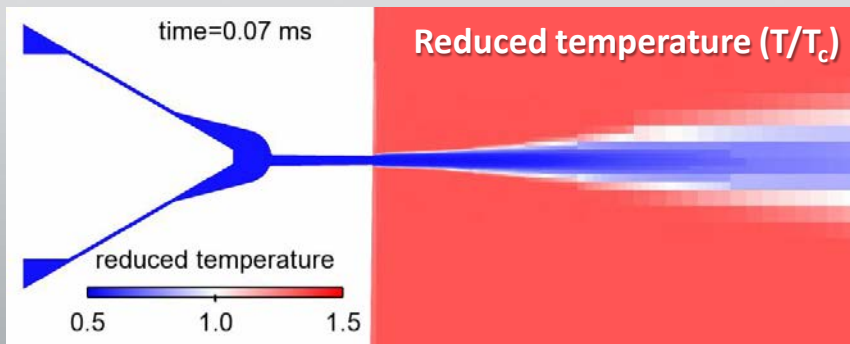
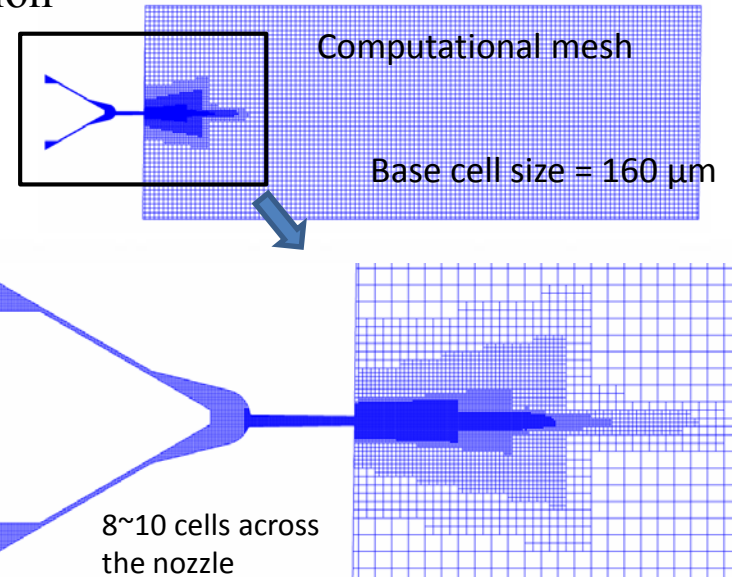
Incorporate developed physical model for liquid properties

- Improve predictions for high pressure and high temperature fuel injection
- Improve understanding of thermodynamics process of in-nozzle flow and fuel-air mixing

Test case for ELSA model under sub-critical condition

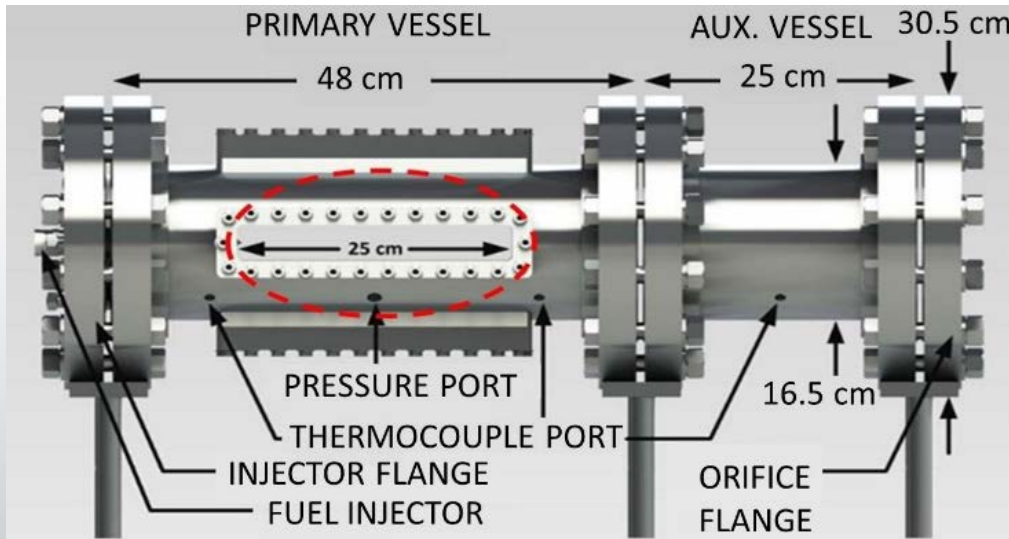
Engine Combustion Network Spray A

| | |
|---------------------------|--|
| Nominal Ambient Temp. | 900 K |
| Nominal Ambient Density | 22.8 kg/m ³ |
| Fuel | n-dodecane (critical point: 658.15 K, 18.17 bar) |
| Injected fuel temperature | 363 K |
| Injection Pressure | 1500 bar |
| Nozzle hole diameter | 89 μm |
| CFD Software | Converge 2.3 |
| Liquid properties | Converge predefined fuel library (only temperature-dependent) |



- Super-critical with respect to pressure **BUT** sub-critical with respect to temperature for the liquid fuel

Subcritical Experimental Results



- Continuous flow of compressed preheated air (subcritical)
- N-heptane is supplied by Bosch CRIN3-18 Injector, modified with single 100 μm orifice
- Injection duration: 4 ms, 12 injections per minute

- n-heptane
- Fuel supply pressure of 1000 bar
- Chamber air temperature of 180 C
- Chamber pressure of 13 bar
- Schlieren field of view is about 60 mm
- Mie-scatter images were acquired at same conditions

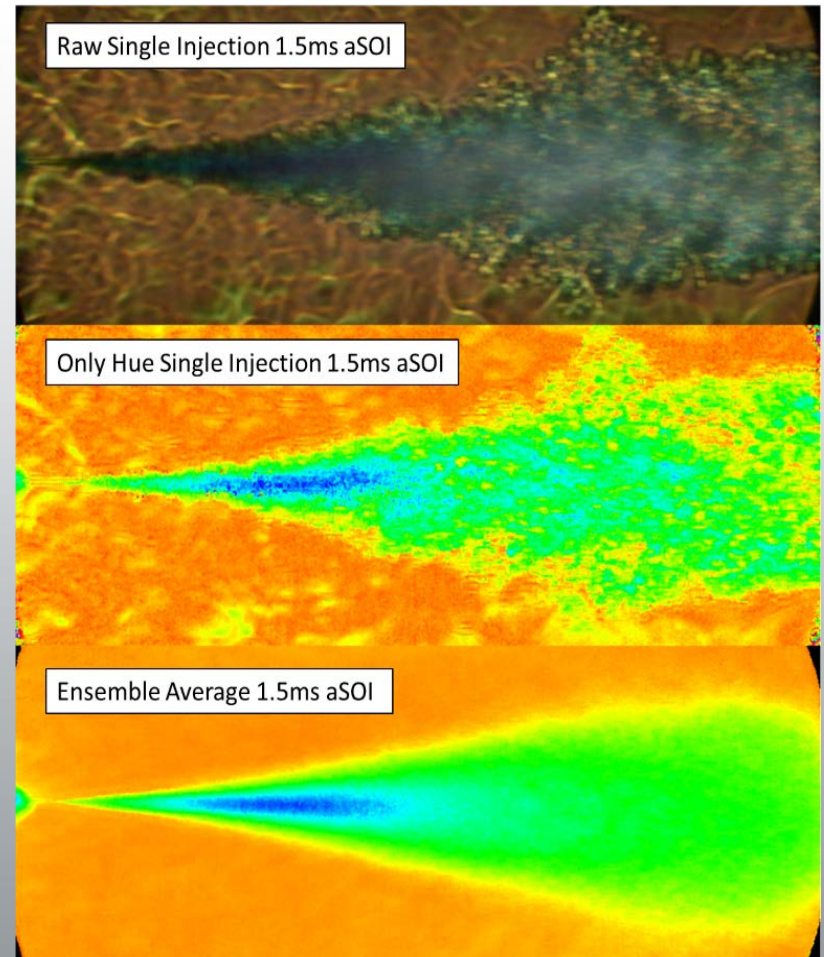
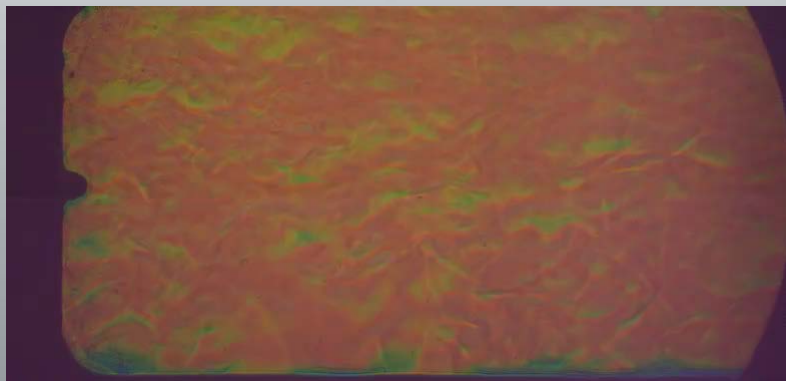
Rainbow Schlieren Images

Imaging Setup

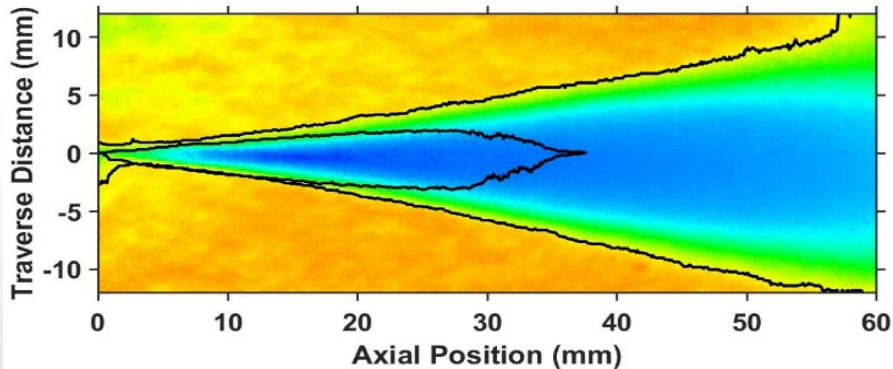
- Exposure time: 4 μ s
- Framing rate: 10 kHz
- Spatial resolution 83 μ m/px

Image Processing

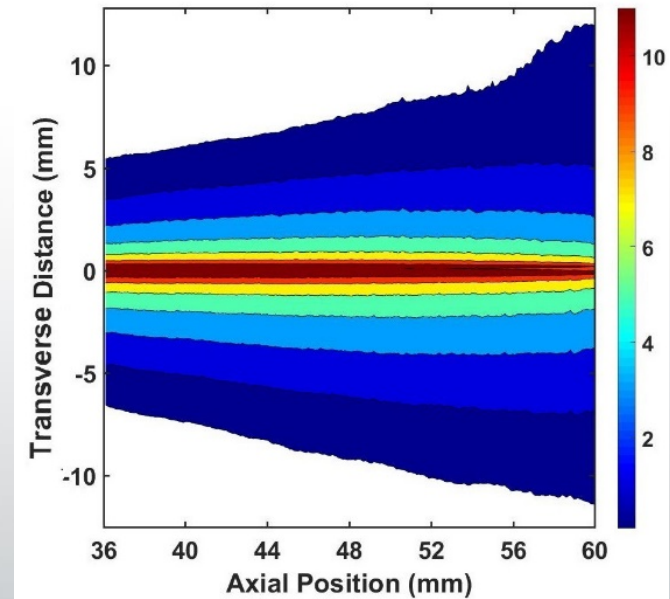
- Color is quantified by Hue
- Instantaneous images
- Ensemble averaged image



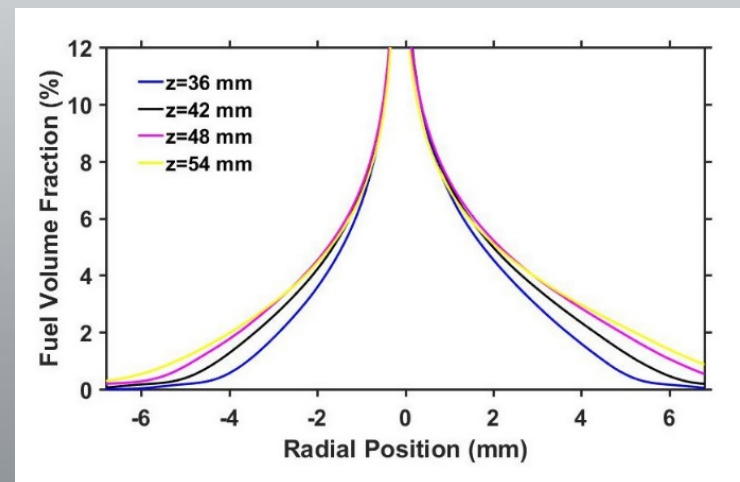
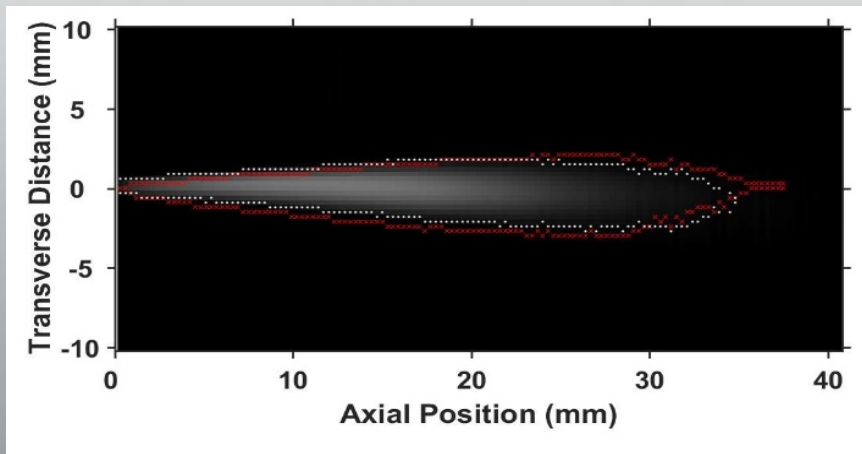
Liquid Core Length

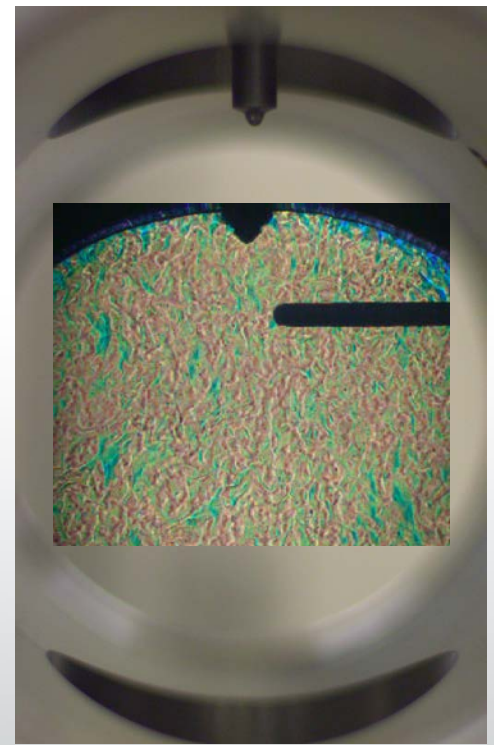
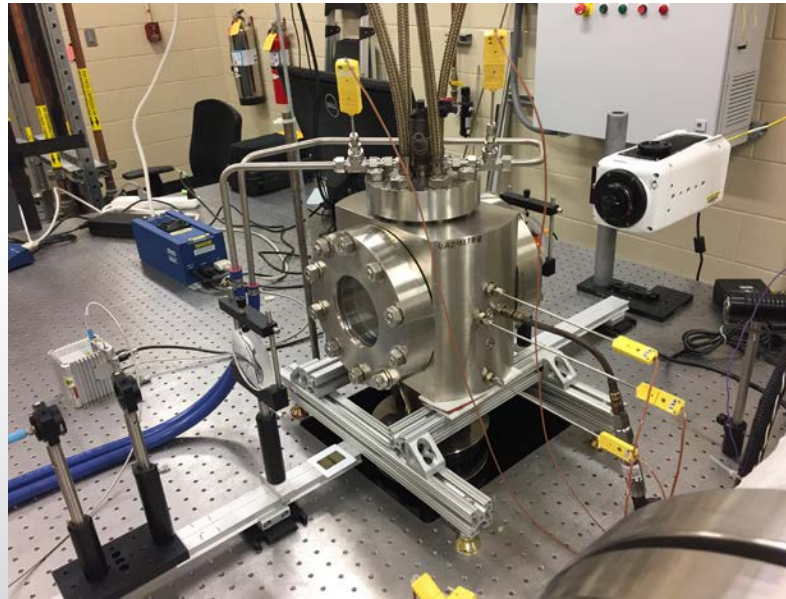
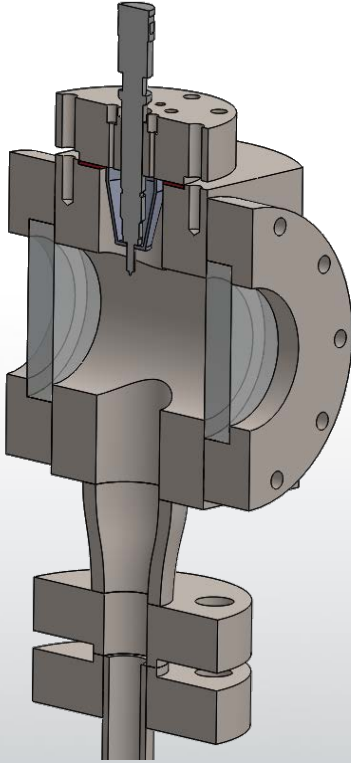


Fuel Volume Fraction



Comparison with Mie-scattering





Designed and fabricated a constant pressure test chamber for fuel injection and mixing at supercritical conditions

- Up to 50 bar, 1000 K
- Counter-flow design
- Injector cooling provided with water jacket
- 12 injections per minute once stable

- CPFR successfully tested and operated
 - 34 bar, 1100 K heater set point.
 - 825 K near injector.
 - Injector cooling jacket, 90°C
- Corresponding Reduced Temperature/Pressure
 - Heptane, $T_r = 1.5$, $P_r = 1.25$
 - Dodecane, $T_r = 1.25$, $P_r = 1.8$
- Sample image shows a sample color schlieren image with 1/8" thermocouple visible

Collaboration and Coordination

- Project represents a partnership between The University of Alabama, UA (prime) and Argonne National Laboratory, ANL (sub).
- UA is providing expertise in two areas:
 - Development of property models and related software
 - Experimentation and optical diagnostics in a constant pressure flow rig

We consult with Sandia National Lab to ensure safe and reliable operation of the test chamber. We work with ANL to implement property models in CFD software
- ANL is providing expertise in:
 - Computational fluid dynamic analysis of diesel sprays
 - Large scale computing

ANL is working with the developers of the commercial software code CONVERGE
- UA and ANL hold technical meetings on a monthly basis to coordinate experimental and computational efforts.
- The research team holds project meetings with project/technical monitors on a quarterly basis.

Remaining Challenges and Barriers

- Evaluate the effect of pressure on thermal conductivity
- Evaluate the mass diffusivity model(s)
- Implement property models in CFD code to perform fuel-air mixing calculations for a simplified test case
- Debug and validate the CPFR facility to acquire reliable schlieren measurements
- Analyze schlieren images to infer quantitative data on fuel-air mixing
- Compare experimental and computational results and resolved any discrepancies found
- Perform parametric analysis: experimentally and computationally

Proposed Future Research

- Conduct preliminary and baseline experiments in the modified CPFR
- Conduct parametric experimental study
- Evaluate the proposed EE approach with real-fluid model using an open source CFD code
- Evaluate the proposed EE approach with real-fluid model using a commercial CFD code
- Integrate the developed models into a commercial CFD code and perform validation and demonstration studies
- Document and disseminate validated source codes

Any proposed future work is subject to change based on funding levels

Summary

Relevance

- This project will acquire experimental data, and develop property models to accurately model fuel-air mixing at supercritical conditions for diesel application using open source and commercial CFD codes

Approach

- Innovative rainbow schlieren deflectometry optical diagnostics technique is used to acquire quantitative data in a constant pressure flow rig
- Detailed models to calculate thermodynamic properties are developed and implemented in CFD software, and validated.

Technical Accomplishments

- Developed and validated fluid property models using NIST database
- Identified test case, and coordinated to implement property models in CFD code
- Designed and constructed a constant pressure flow rig
- Implemented and validated schlieren diagnostics techniques

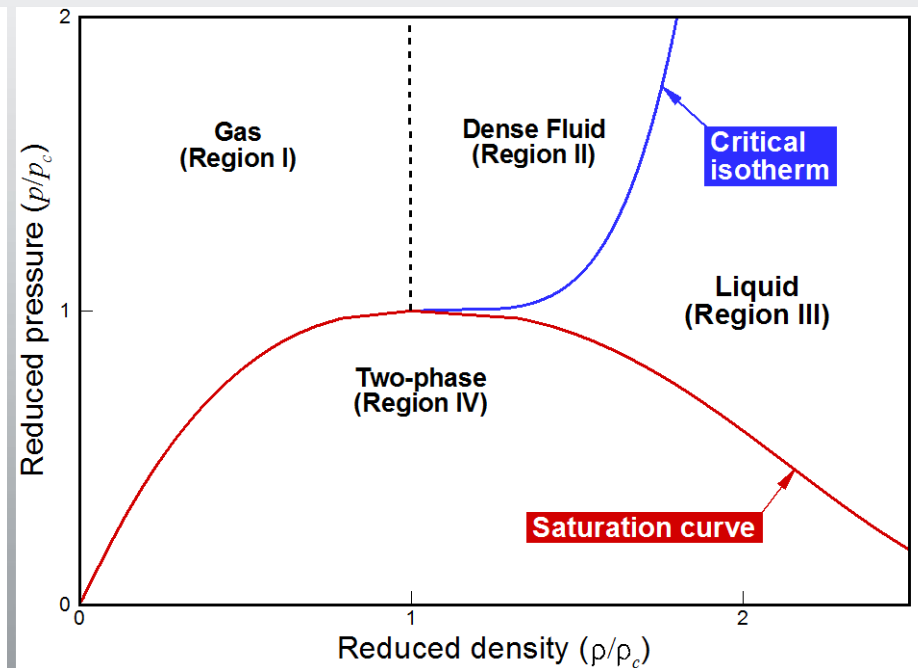
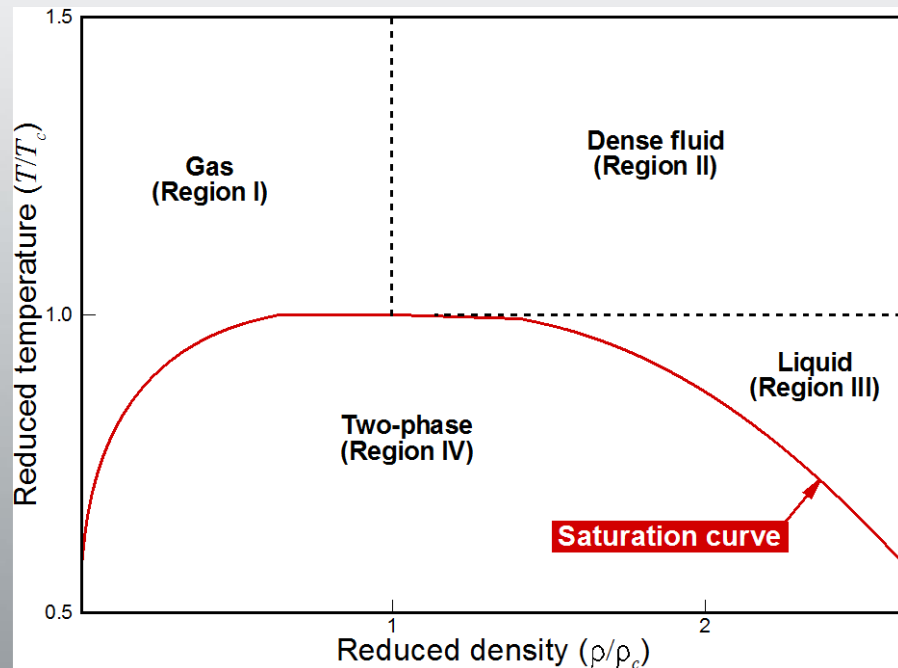
Future Work

- Implement property models in CFD software
- Acquire test data in the flow rig
- Compare experimental and model results to resolve any discrepancies
- Conduct parametric analysis

Technical Backup Slides

Thermal Property Models

- Specific sub-models depend on regions as defined:



Thermal Properties

- The following correlations/models were selected for calculating thermal properties
 - Pitzer's correlation for saturation pressure
 - For saturated liquids, Rackett's model (1970), Lee-Kesler model (1975), Spencer-Danner correlation (1972), Yamada-Gunn model (1973), and model by Polling, et al. (2000) were selected
 - For saturated vapor, Carruth-Kobayashi model (1972) and Watson model (1943) were employed
 - For the region of gas, the modified van der Waals equation was used
 - For the regions of liquid and dense fluid, the HBMS (Hirschfelder, *et al.* 1958) was employed
 - For the two-phase region, a fluid "quality" was calculated based on the known volume and its linear interpolation between saturated gas volume and liquid volume

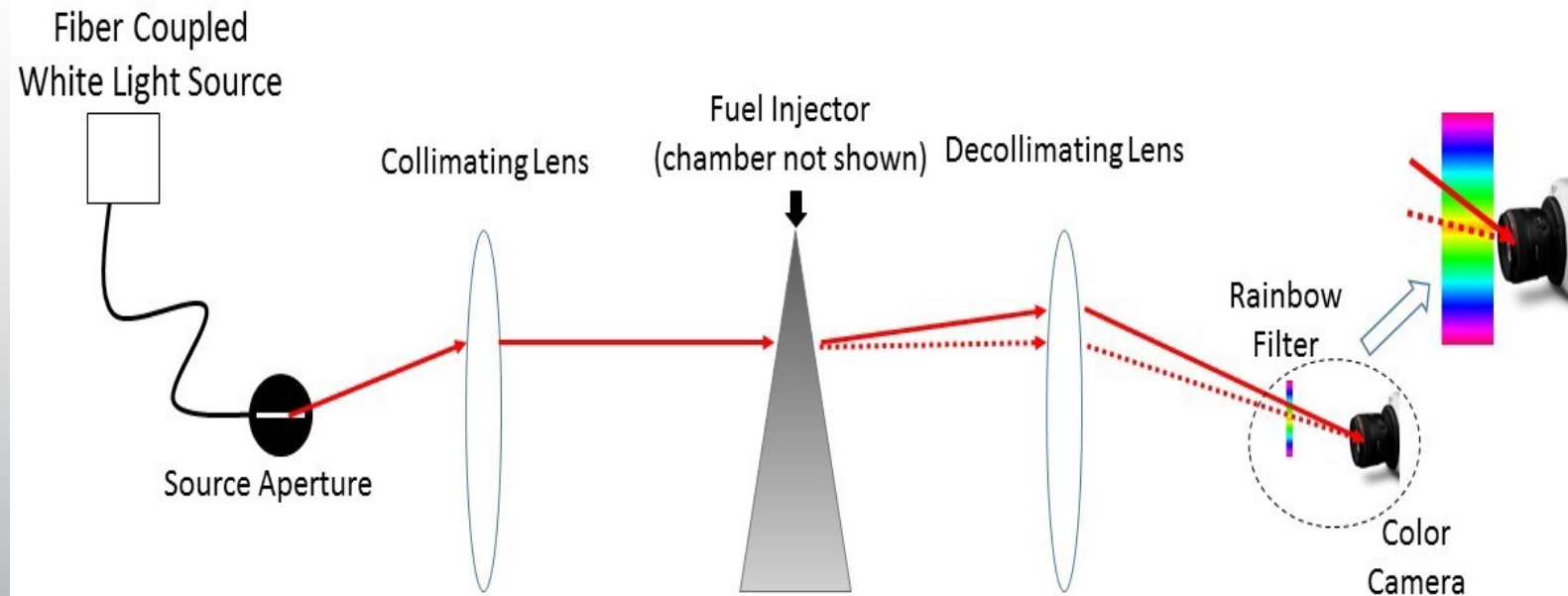
Viscosity

- The corresponding states approach was selected for modeling the fluid viscosity instead of the Chapman-Enskog theory because of its applicability of wide range of thermodynamic states
- The corresponding states methods for modeling fluid viscosity are divided into 4 categories:
 - Low-pressure gas region (Lucas [1980])
 - Low-pressure liquid region (Reid, *et al.* [1987] and modification of Letsou and Stiel [1973])
 - Pressure effect on gas viscosity (Lucas [1980, 1981])
 - Pressure effect on liquid viscosity (Lucas [1981])

Thermal Conductivity

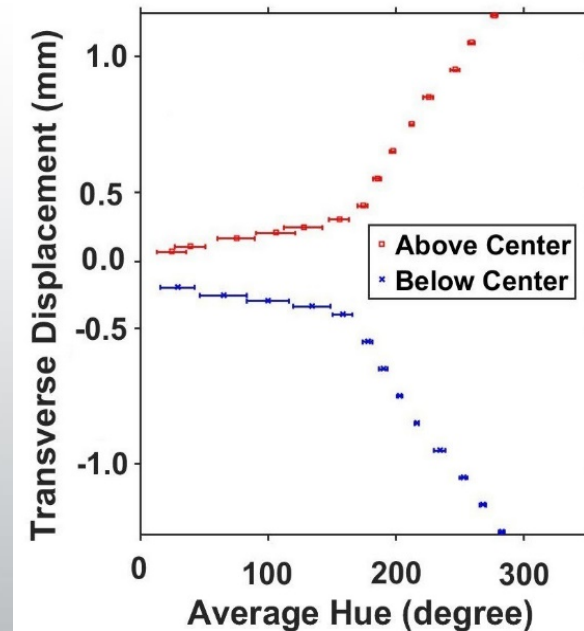
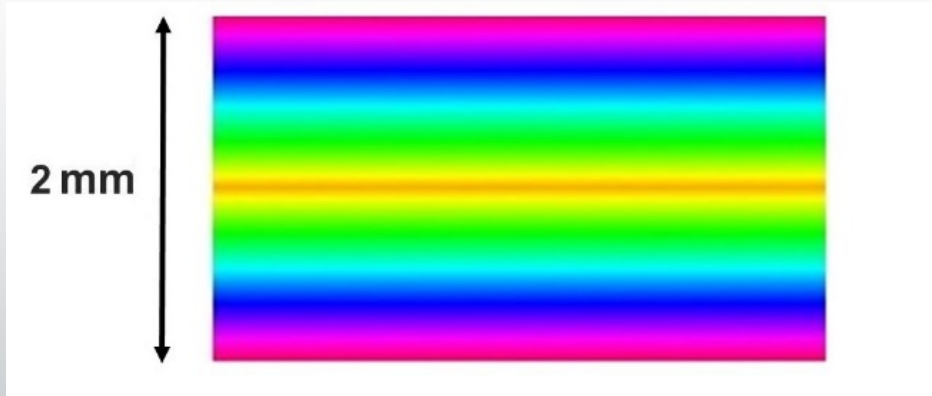
- The corresponding states approach was selected for modeling the fluid thermal conductivity because of its applicability of wide range of thermodynamic states
- The corresponding states methods for modeling thermal conductivity are divided into 4 categories:
 - Low-pressure gas region (Chung, *et al.* [1984] [1988])
 - Low-pressure liquid region (modification of Sastri [Poling, *et al.*, 2001])
 - Pressure effect on gas thermal conductivity is under investigation
 - Pressure effect on liquid thermal conductivity is under investigation

Rainbow Schlieren Deflectometry (RSD)



- High-intensity, fiber coupled white light source, rectangular source aperture, collimating and decollimating lenses
- Rainbow filter, high-speed camera

Rainbow Filter



- Deflected rays pass through different colors on the filter.
- Filter serves as a ruler to measure the deflection of light rays, which is related to density or equivalence ratio.

Publications and Presentations

- Christopher Wanstall, Ajay K. Agarwal, and Joshua Bittle, “Quantifying liquid core of a fuel spray by rainbow schlieren deflectometry,” *Applied Optics*, in review.